



## Developing an interface between MCNPX and McStas for simulation of neutron moderators

Lauritzen, Bent; Nonbøl, Erik; Klinkby, Esben Bryndt; Willendrup, Peter Kjær

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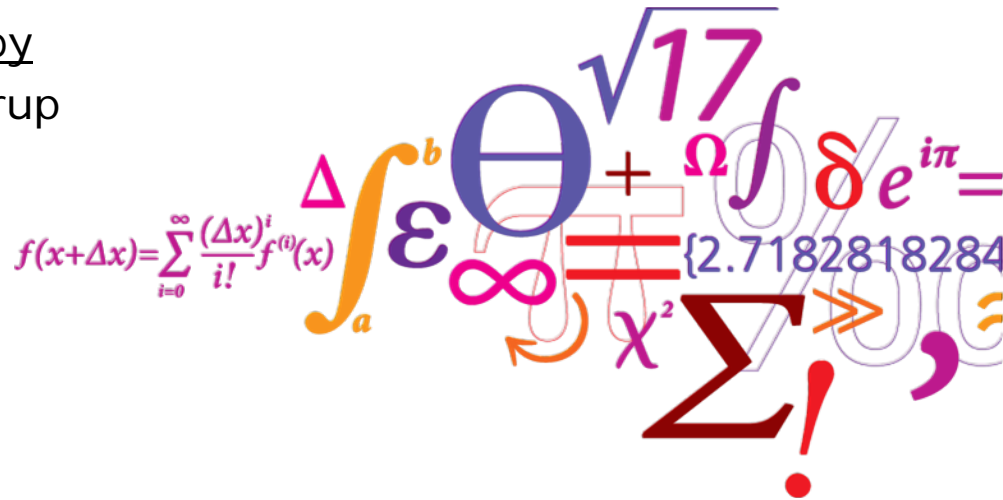
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# Developing an interface between MCNPX and McStas for simulation of neutron moderators

Bent Lauritzen  
 Erik Nonbøl  
Esben Klinkby  
 Peter Willendrup





# Motivation

- Traditionally two decoupled Monte Carlo codes covers different needs in Neutron Scattering simulations:
  - MCNP/X used for TMS calculations
  - Neutron ray tracing code, e.g. McStas (talk by P. Willendrup) used for instrument design + data analysis
- Even more precise simulations may be possible by combining the best of the two worlds: The detailed description of incoherent scattering from MCNP/X with the coherent scattering of McStas.
- **Prospects:** usage of direct MCNP/X McStas coupling:
  - Optimization of complex moderator design
  - Shielding along neutron guide
  - Crosstalk between neutron guides
- Test case: ESS TMS and guide systems.



# Outline

## ➤ Explored interfaces:

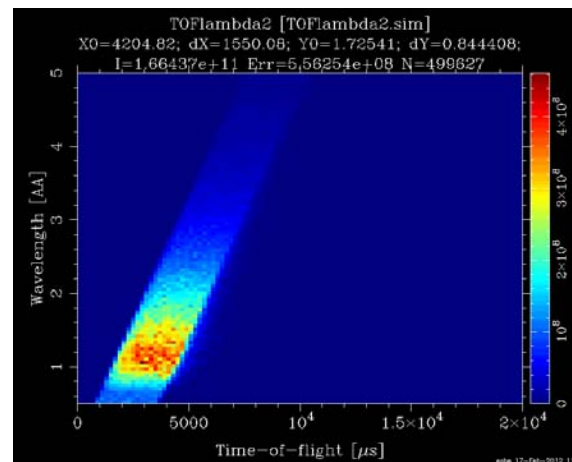
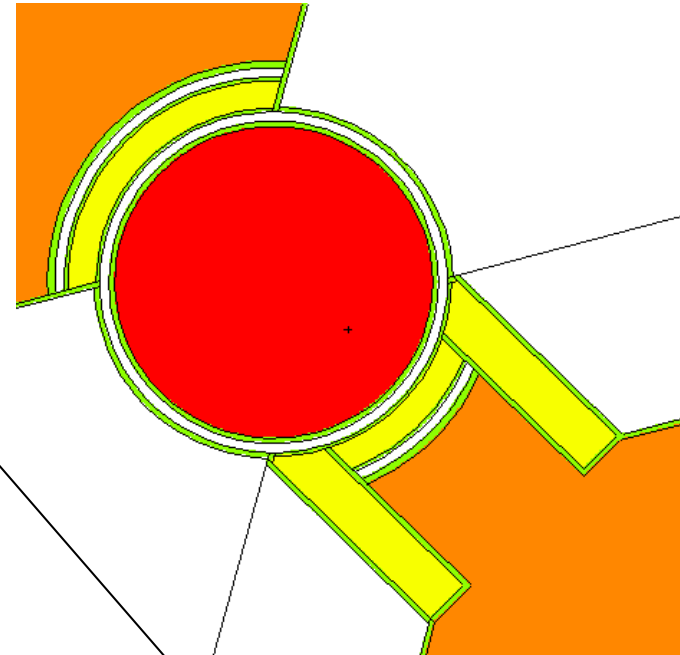
- Tally fit
- Ptrac
- SSW/SSR
- Compile
- Supermirror

## ➤ Validation

- First results
- Upcomming

## ➤ Summarizing experiences

- Cross comparisons



# Tally fitting (present default approach)

1. Neutron spectrum calculated with MCNP/X at the moderator surface
2. Spectrum is approximated by simple functions which serves as input to McStas.



## Con's

- Correlations (e.g. E, pos, angles) unaccounted for
- No re-entry (format is write-only)

← Discussed later



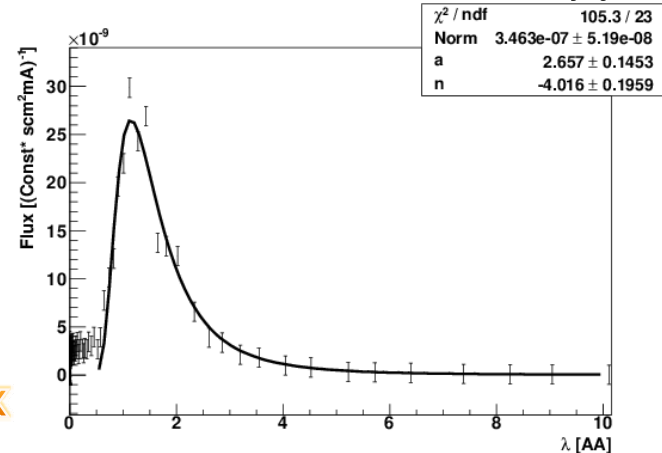
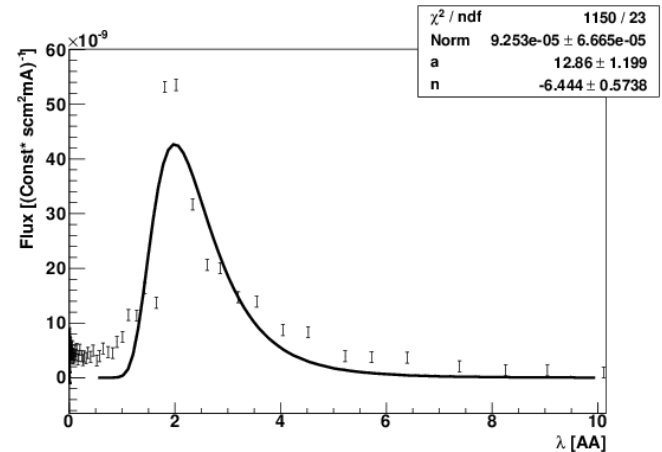
## Pro's

- Fast - MCNP calculation done once-and-for-all
- Avoids licensing issues

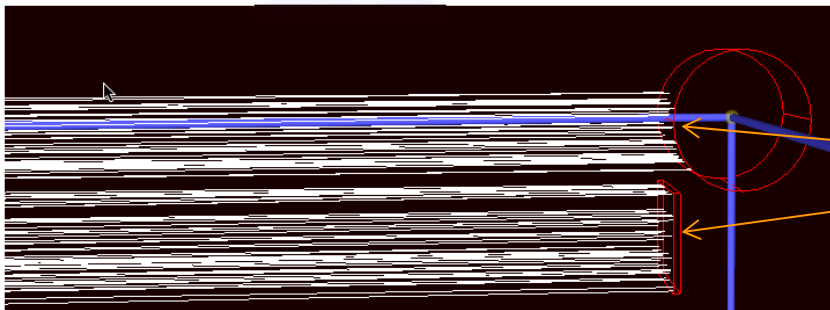
# Tally fitting (update)

➤ Based on the latest MCNPX ESS target station (bi-spectral) geometry from ESS-Bilbao (see presentation by F.Sordo), we have developed a McStas component mimicking both geometry and spectra.

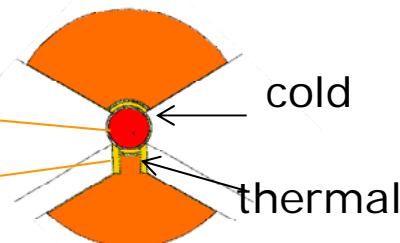
➤ The component is named:  
 ➔ *ESS\_Moderator\_revised*, and is expected to be released shortly.



MCSTAS



MCNPX



# Ptrac

- MCNP/X can output an ascii file containing individual neutron states: pos, angles, energy, time & weight
- The McStas component: *MCNP\_Virtual\_Input* converts the neutron state into McStas readable and works as a source



## Con's

- ascii file enormous: ~0.2kB/evt
- Write out at 1 surface only
- No re-entry (format is write-only)
- Cannot run MPI



## Pro's

- Correlations conserved (e.g. E,pos)
- Fast

## Ptrac format

```

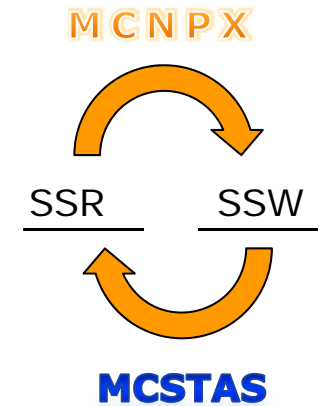
.....
3000      2      10      179
100       2       0
      0.00000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.33356E-02
      3000      3      110      179
10       2       0
      -0.20000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.40028E-02
      3000      4      120      179
100      2       0
      -0.40000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.46699E-02
      3000      5      130      179
.....

```



## SSW/SSR

- Source **S**urface **R**ead/**W**rite in MCNPX starts/stops simulations at a given (set of) surface(s)
- The neutron state written to binary file.
- New McStas components:
  - ➔ *MCNP\_Virtual\_ss\_Input* & *MCNP\_Virtual\_ss\_Output* reads MCNPX output and writes MCNPX input
- Neutron propagation started in MCNPX, continued in McStas and finalizing in MCNP



- ascii file sizable: ~0.1kB/evt
- Write out at selected surfaces only



- All McStas functionality usable
- Re-entry supported
- Correlations conserved (e.g. E,pos)
- Works with MPI

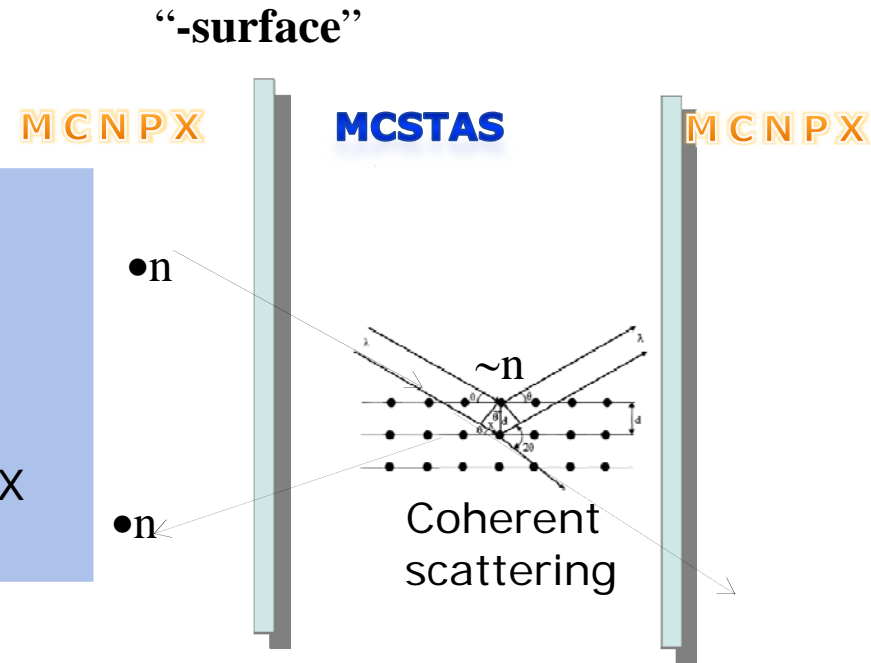




# Combined compilation

## METHOD

- McStas surface flag introduced in MCNPX
- Neutron crossing McStas surface causes initiation of McStas simulation, based on neutron state.
- Updated neutron state returned to MCNPX



- Licensing issue
- Slow: MCNPX called for each neutron



- Potentially very flexible (but not yet fully developed)
- All McStas functionality usable
- Re-entry supported
- Correlations conserved (e.g. E,pos)

in MCNPX input file:

.....

-110 PX -0.2

-120 PX -0.4

.....

# Supermirror

➤ Existing implementation, introducing McStas inspired supermirrors as a surface card in MCNPX (Gallmeier et al, Nuc.Tech. 168(3))

➤ Reflectivity  $R=R_0$   $if\ Q < Q_c$

➤  $R=R_0/2\{1 - \tanh[(Q - mQ_c)/W]\}\{1 - a(Q - Q_c)\}$   $if\ Q \geq Q_c$

➤ Ported to MCNPX 2.7, but not yet validated



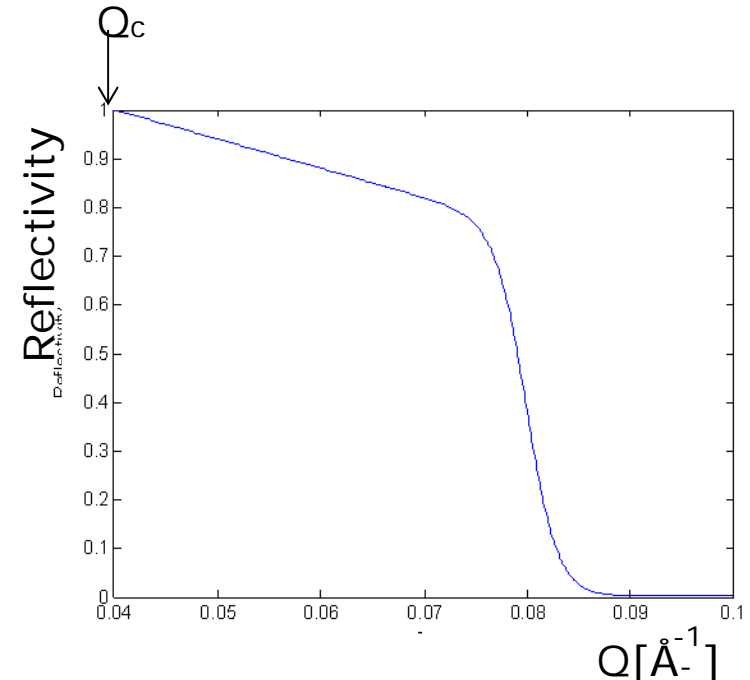
Doesn't scale: workload per functionality significant. Only McStas mirrors ported

- Licensing issue
- Slow



Re-entry supported

- Correlations conserved (e.g. E,pos)
- Avoids intermediate files and multiple codes



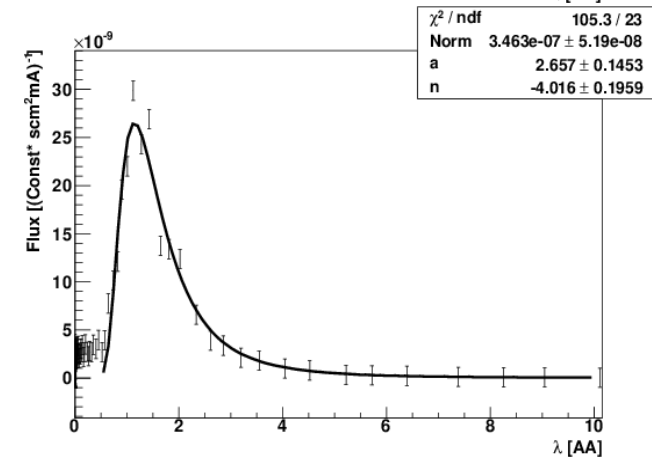
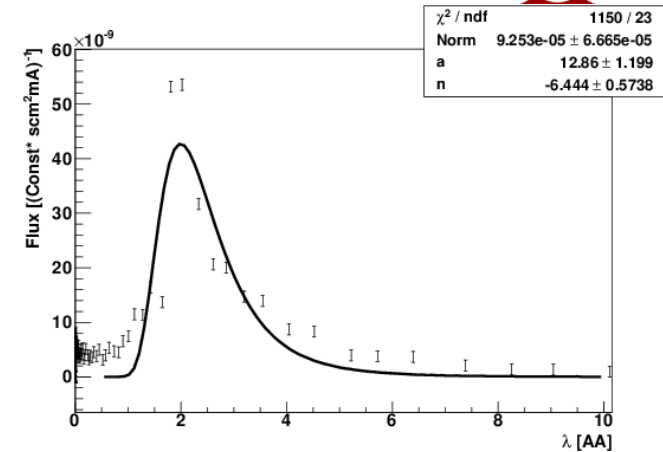
# Validation:

## Fitting distributions vs. importing neutron states

- Present approach used for instrument design & physics analysis relies on a once-and-for-all fit to a spectrum.
- Clear advantages over porting individual neutrons:
  - Preliminary ESS geometry (from ESS-Bilbao), simulation 1M protons with MCNPX takes ~1K CPU hours
  - McStas CPU cost for 1M neutrons: hardly measureable <1s
- Implicitly McStas assumes:
  - Spectrum fit is perfect
  - No correlations between: Position at moderator surface, position at guide entrance, momentum
  - No scattering between moderator surface and guide entrance
- For TMS & instrument design these assumptions are worth questioning

# Validation of Tally approach: Fits

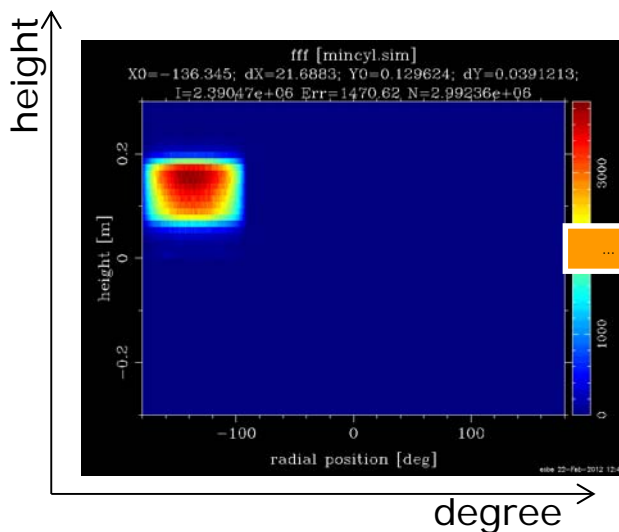
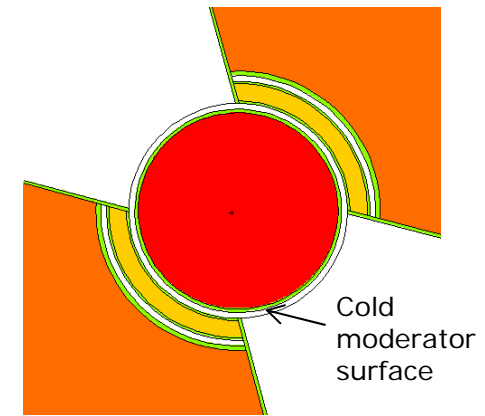
- No fit is ever perfect – especially not mine



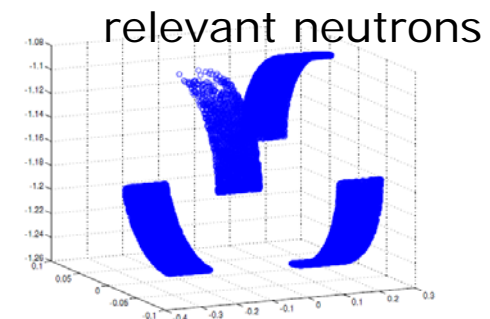
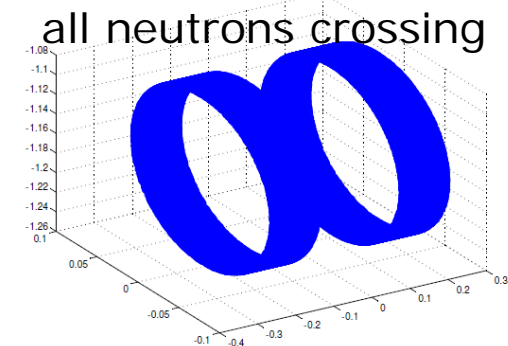
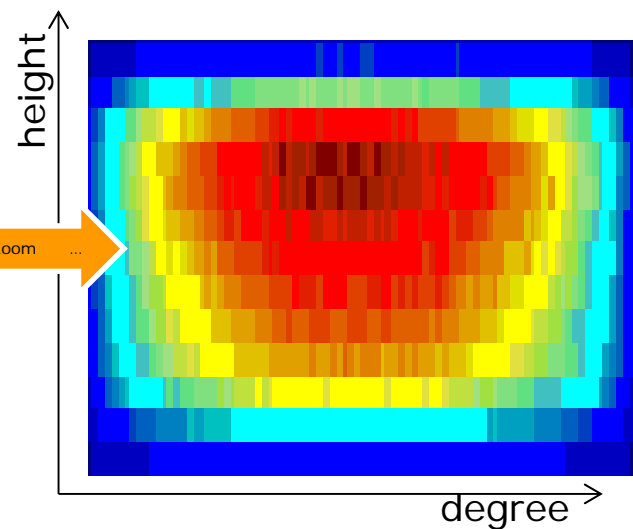
# Validation of Tally approach: Correlations

Stress test of the developed SSW/SSR approach:

- Simulate 1M protons hitting target wheel
- Dump all neutrons passing moderator surface to SSW output file (3.5Gb)
- In McStas, placing a **PositionSensitiveDetector** (PSD) ~at the cold moderator surface gives:

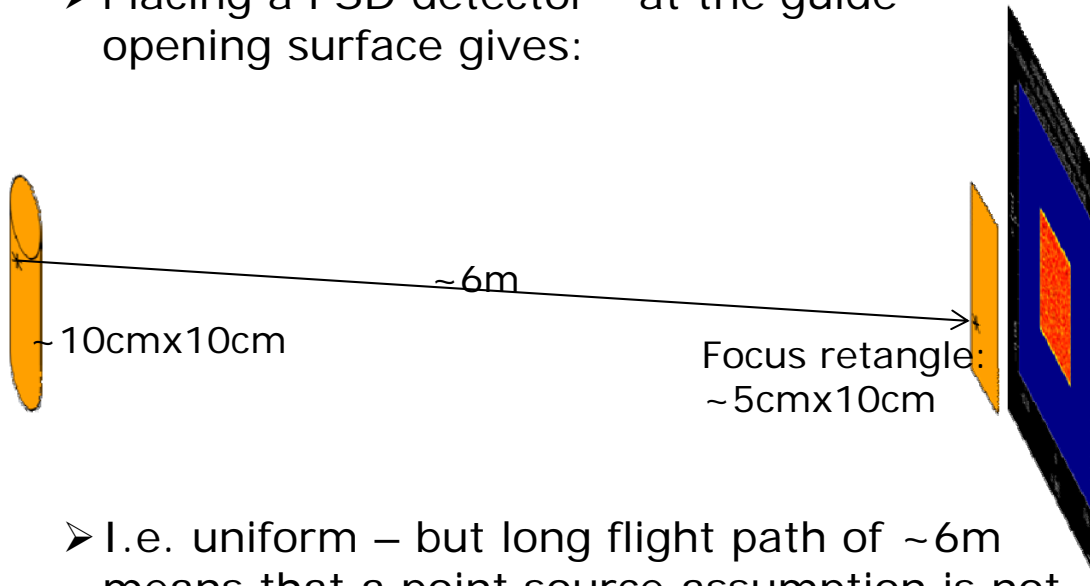


... Zoom ...

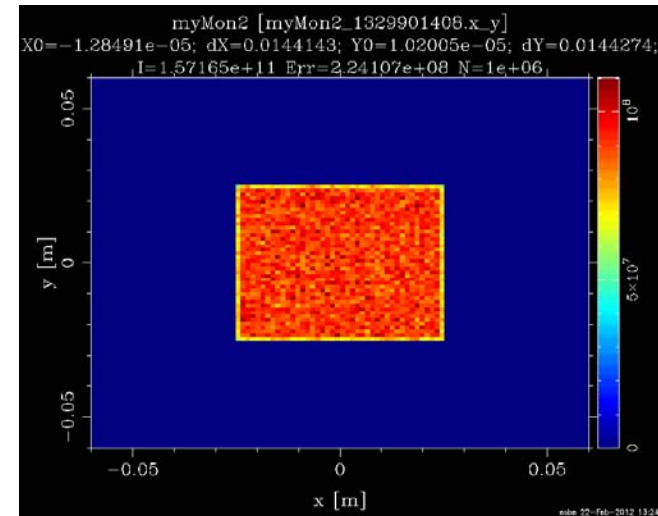


# Validation of Tally approach: Correlations

- In McStas the procedure to provide neutron states is to connect randomly points at the moderator to points at the guide opening, and assign energy
- Placing a PSD detector ~at the guide opening surface gives:

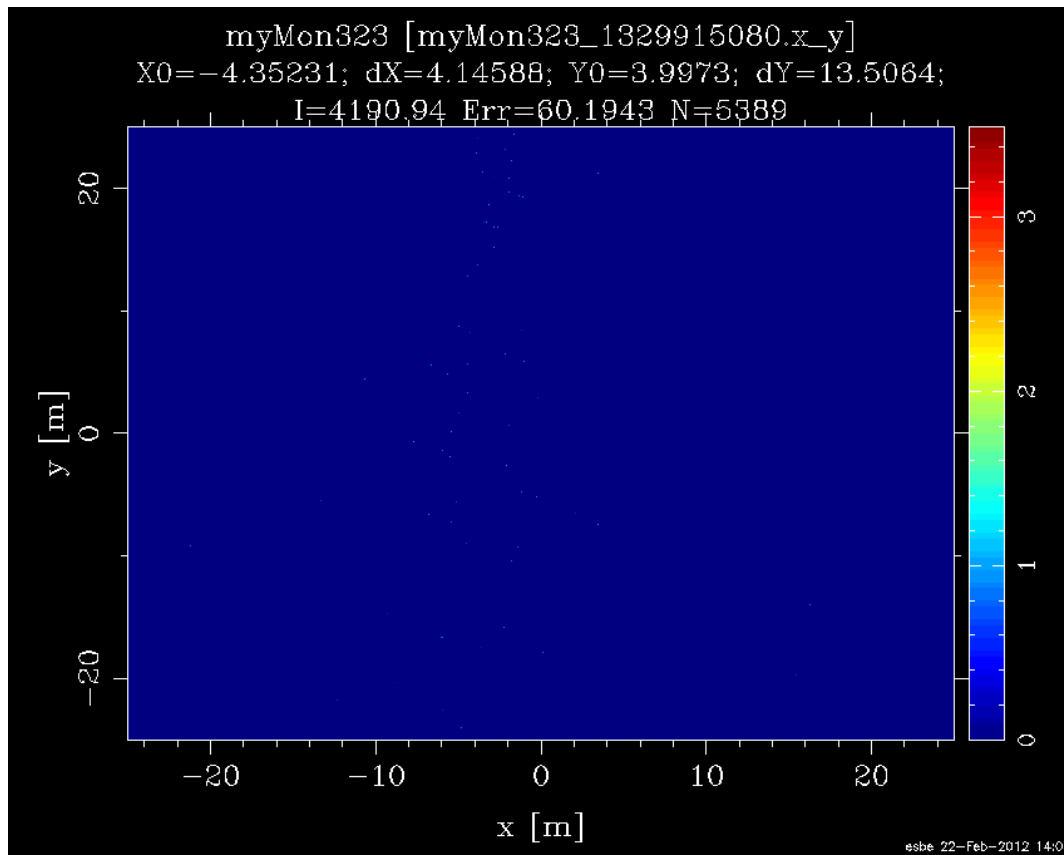


- I.e. uniform – but long flight path of ~6m means that a point source assumption is not too far off.
- **Q:** How would the distribution look in MCNP. I.e. SSW card at 6m?



# Validation of Tally approach: Correlations

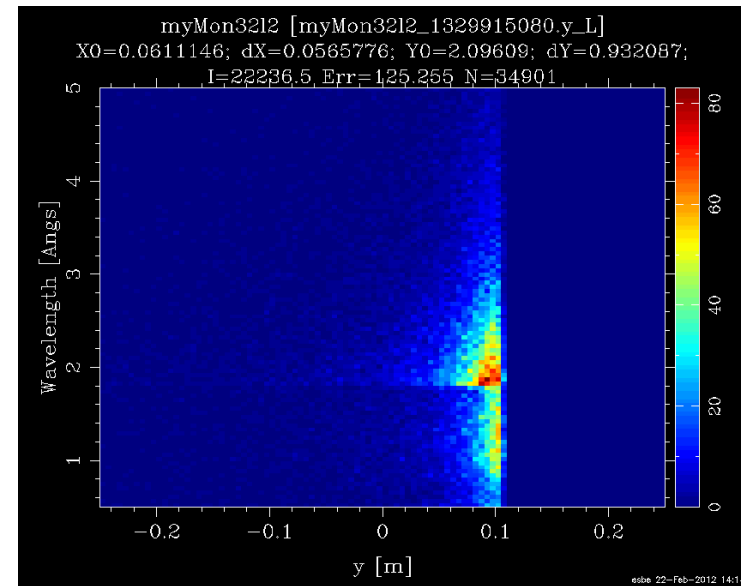
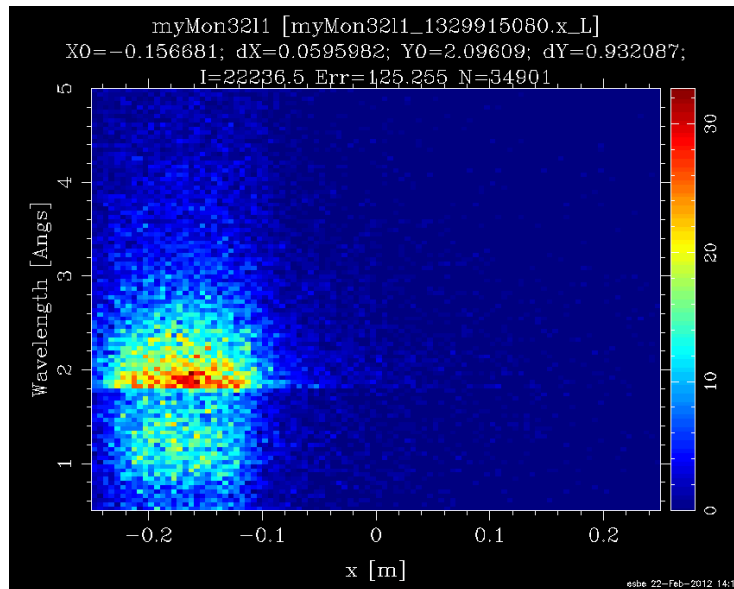
➤ **A:** Flat – in the empty sense of the word:



➤ No focus -> very few neutrons at guide

# Validation of Tally approach: Correlations

- Lots of other comparisons to make:

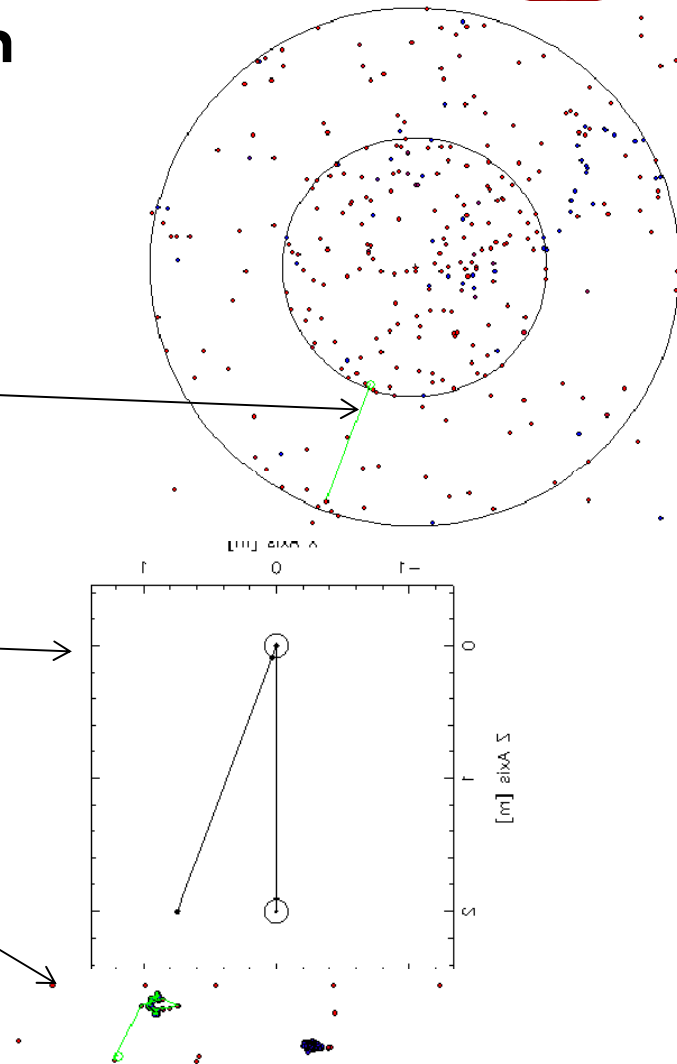


- I.e. correlations between position & energy exist. Important for moderator design etc, but perhaps not for instrument design (?). Being investigated.



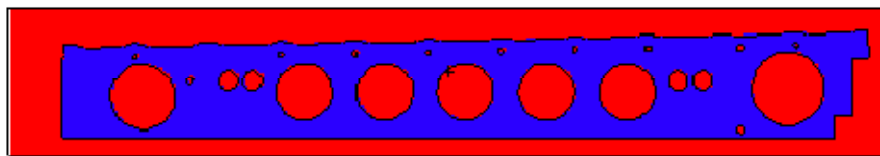
# Validation of SSW / SSR approach

1. Define simplest possible geometry in MCNPX
2. Run test simulation
3. Visualize events and pick one
4. Import to McStas the neutron states as recorded by SSW card
5. Run simplest possible McStas simulation from SSW input: neutron transport
6. At  $z=2\text{m}$ , write SSW & visualize
7. Based on McStas SSW resume the MCNPX simulation, and visualize

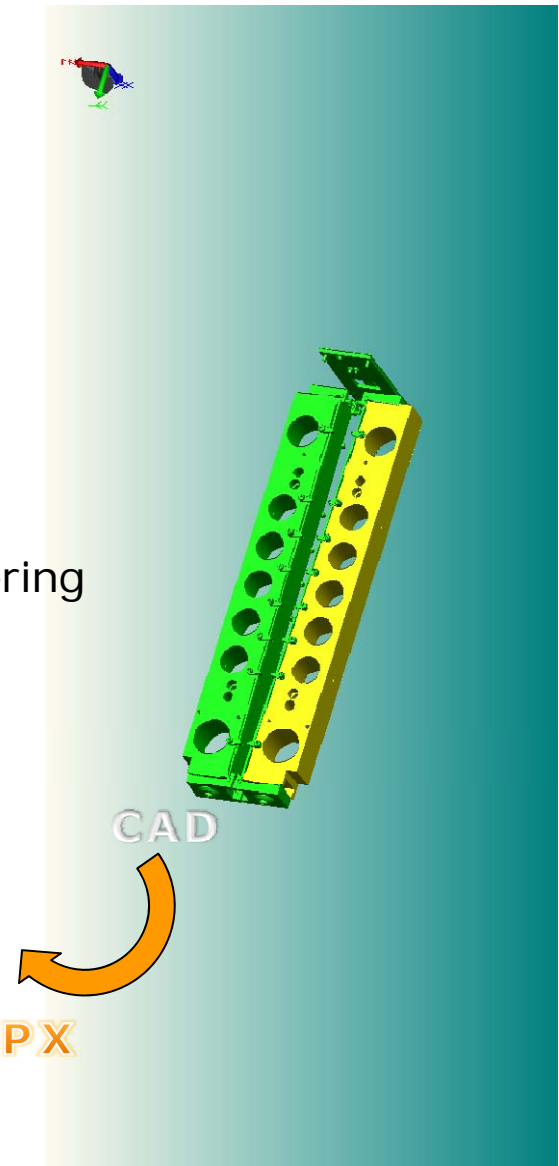


# Validation: upcomming

- Test all interfaces using ESS prototype guide at SINQ spallation source at PSI in summer 2012
- Allows cross validation of simulation approaches against real data
- Status (simulation-wise): Using MCAM<sub>1)</sub> engineering CAD model geometry has been translated into a MCNPX readable geometry (details missing still)



MCNPX



## Cross comparison

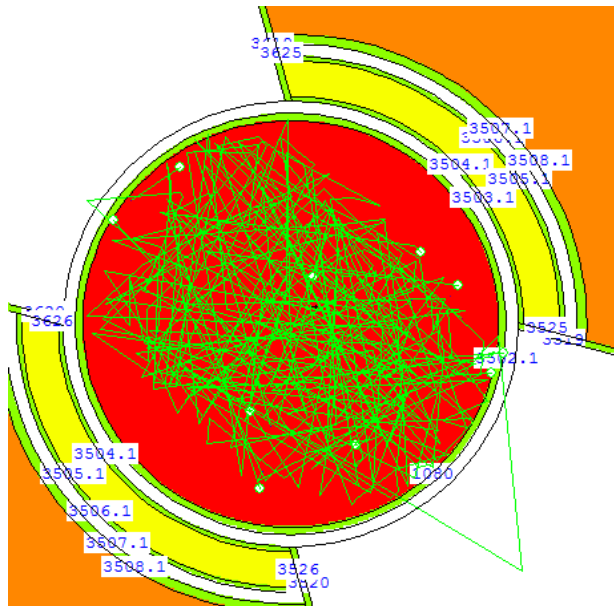
|             | Re-entry neutrons | Speed             | Single neutron trace | Require License | Comments                                       |
|-------------|-------------------|-------------------|----------------------|-----------------|--|
| Tally       | No                | Fast <sup>*</sup> | No                   | Yes/No          | Should try to determine validity at least once |
| Ptrac       | No                | Fast <sup>*</sup> | Yes                  | Yes             | Somewhat outdated by SSW/SSR                   |
| SSW/SSR     | Yes               | Fast <sup>*</sup> | Yes                  | Yes             | Promising...                                   |
| Compile     | Yes               | Slow              | Yes                  | Yes             | Generalizes poorly (auto gen c-code hacks)     |
| Supermirror | Yes               | Slow              | yes                  | yes             | Generalizes poorly (but who cares?)            |

<sup>\*</sup>) The computational heavy MCNP/X calculation can be performed once-and-for-all

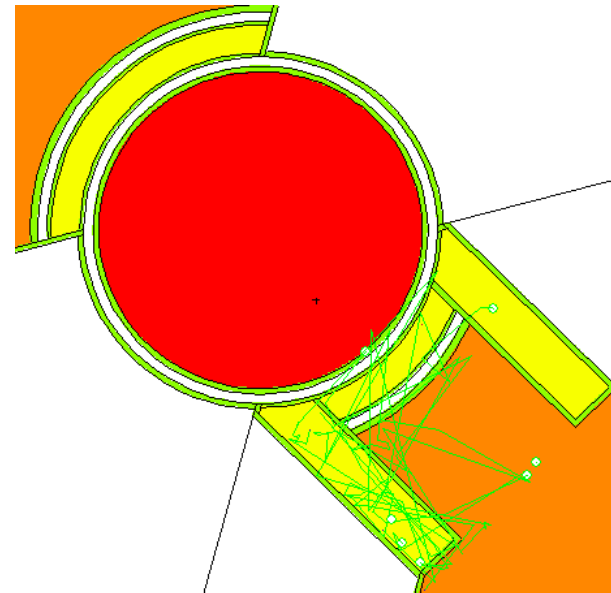
# Backup slides

# Tally contributions

➤ Contributions to cold spectrum



➤ Contributions to thermal spectrum



# Fits

